

Electron linewidths of wide-gap insulators: excitonic effects in LiF

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Based on a recent exchange–correlation kernel developed within Time–Dependent–Density–Functional Theory we derive a practical and general expression for the three–point vertex function. We show that excitonic effects in LiF strongly modifies the low–energy electron linewidths leading to linear scaling with quasiparticle energy. We also prove that, in contrast to previous results for the electron gas, simple metals and semiconductors, vertex corrections in the self–energy and in the screening function do not compensate each other.

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The experimental quasiparticle band structure of bulk metal and semiconductor systems has been successfully explained by the GW self–energy scheme [1, 2, 3] in its simplest non self–consistent G_0W_0 implementation. Similarly, the quasiparticle linewidths of simple and noble metals have been studied extensively [4], but a first–principles description of the electronic contribution to the electron/hole linewidths in semiconductor and insulators is not yet available. The reason is that the low–energy quasiparticle dynamics in semiconductors tends to be dominated by inelastic phonon scattering, the electronic contribution playing a minor role. However this scenario changes drastically when the quasiparticle energy is larger than the minimum energy required to excite an electron–hole pair. Above this threshold (that is zero in metals and approximatively twice the band gap in insulators) the rapidly increase in density of electron–hole pairs dominates the quasiparticle damping, resulting in a mainly electronic contribution to the lifetime. It is well known that in insulators, at difference with metals, the attractive interaction between electrons and holes can lead to the formation of a bosonic–like excitonic state [3]. Excitons modify remarkably the optical and energy-loss spectra and, consequently, the microscopical mechanisms responsible for the quasiparticle damping. This effect is stronger in wide–gap insulators like LiF.

In this communication we tackle the problem of evaluating the impact of the excitonic effects on the quasiparticle (QP) dynamics of LiF, using a simplified vertex function in the electronic self–energy. An efficient approximation for the *three–point* many–body vertex function is given in terms of the *two–point* exchange–correlation kernel f_{xc} [5], recently developed in the framework of Time–Dependent–Density–Functional Theory (TDDFT) [3]. As result we show that the electronic linewidths of LiF display a linear dependence as function of the QP energy, that can be traced back to the incipient excitonic effects induced by f_{xc} [6]. Understanding the inelastic mechanism which dominates the phase coherence time is crucial to the field of quantum transport in mesoscopic and nanostructured materials. Thus this

work is the first steps toward a full first–principles description of the quasiparticle dynamics of semiconductor and insulators.

In the usual one–shot G_0W_0 self–energy scheme, it is assumed that a basic Density–Functional–Theory (DFT) calculation [7] provides good approximation for QP wavefunctions and electronic screening (dominated by collective excitations, plasmons build from independent electron–hole transitions, i.e. excitonic effects in the screened Coulomb potential W_0 are neglected). The QP lifetime τ_i can be calculated with the Fermi golden–rule, using this non interacting W_0 as scattering potential: $\tau_i^{-1} = -2 \sum_f |\Omega_{if}|^2 \text{Im}[W_0(E_i - E_f)]$, where $|i\rangle$, $|f\rangle$ are the initial and final state, with W_0 matrix elements Ω_{if} , and energies E_i E_f such that $E_i - E_f > 0$. This scattering scheme, also known as “on–mass shell” approximation to the G_0W_0 linewidths, provided valuable insight into the electron/hole linewidths of metals [4]. Therefore, in Fig. 1 we estimate the electronic line widths of LiF (boxes) within this approximation. As W_0 is calculated in terms of non–interacting electron–hole pairs $\tau_i^{-1} = 0$ when $E_i - E_f < E_{gap}$ (E_{gap} the DFT gap): quasiparticle states with energy $E_i < 2E_{gap}$ have zero line width (infinite lifetime). These states are indicated by the dashed area in Fig. 1. Above this region a quadratic energy dependence of the line width is recovered, as in metals [8].

As the short–range screened Coulomb repulsion modifies drastically the polarization function in LiF, one is tempted to apply the previous “on–mass shell” scheme to analyze the role of excitonic effects on the quasiparticle dynamics. This would correspond to replace W_0 by the screened coulomb potential W obtained from the many–body Bethe–Salpeter equation (BSE) [3, 9, 10]. In practice, the BSE sums all the possible binary collisions between electrons and holes, providing a consistent and successful framework for the calculation of the interacting polarization function. However, the BSE is computationally very demanding and it becomes unpractical when the microscopical dielectric matrix $\hat{\epsilon}(\mathbf{q}, \omega)$ must be calculated for a large set of transfer momenta \mathbf{q} and frequencies ω , as

it is the case for the calculation of linewidths [4]. To bypass this difficulty we compute $\hat{\epsilon}(\mathbf{q}, \omega)$ within a TDDFT framework, using an f_{xc} kernel [5] that mimics well the BSE results [11]. This performance is illustrated in Fig. 2 for the loss function $\hat{\epsilon}^{-1}(\mathbf{q}, \omega)$, that is the relevant quantity to build the screened Coulomb potential W . From Ref. [5] we know that TDDFT reproduces the experimental loss function, therefore comparing the TDDFT and random phase approximation (RPA) results of Fig. 2 we see that RPA misses the strong weight of the loss spectra just above the band-gap. Consequently the inclusion of excitonic effects in this G_0W calculation translates into a drastic change of the quasiparticle decaying rates (red circles in Fig. 1) compared to the RPA results (blue boxes).

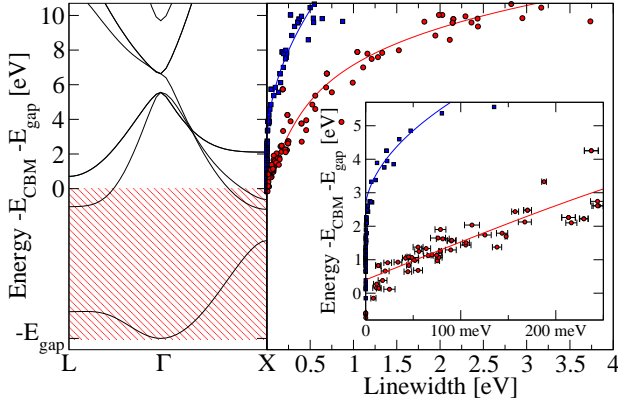


FIG. 1: (Color on-line) Left panel: calculated DFT band-structure of LiF (here E_{CBM} and E_{gap} stand for the DFT conduction band minimum energy and the energy gap). Right panel: Electron linewidths calculated “on mass-shell” as function of the single-particle energy. Boxes: RPA G_0W_0 . Circles: TDDFT-based vertex correction to the self-energy, i.e., a $G_0W\tilde{\Gamma}_{TDDFT}^{(1)}$ approach that turn out to be very close to a simpler G_0W calculation (see text). The dashed area denotes the forbidden energy region for quasiparticle decay into electron-hole pairs. Error bars represent the theoretical uncertain due to the “zero-broadening” extrapolation [11].

This simple scattering approach, though appealing, lacks of theoretical consistency. Exchange-correlation effects have been included *only* in the polarization function, while, in the spirit of the original work of Hedin [1], they should be included in the self-energy as well. However we will show below that the results obtained within a proper treatment of self-energy and polarization effects do not deviate appreciably from the previous G_0W results. We start the derivation from the definition of the self-energy operator $\Sigma(1, 2)$, given by [9]

$$\Sigma(1, 2) = i \int d34 W(1^+, 3) G(1, 4) \tilde{\Gamma}(4, 2; 3). \quad (1)$$

Here $G(1, 2)$ is the interacting Green’s function and $\tilde{\Gamma}(1, 2; 3)$ the irreducible vertex function (numbers stands for space, time and spin coordinates). The screened

Coulomb interaction W is: $W(1, 2) = v(1, 2) + \int d34 v(1, 3) \tilde{\chi}(3, 4) W(4, 2)$ where $v(1, 2)$ is the bare Coulomb interaction and $\tilde{\chi}$ the irreducible polarization function:

$$\tilde{\chi}(1, 2) = -i \int d34 G(1, 3) G(4, 1) \tilde{\Gamma}(3, 4; 2). \quad (2)$$

Thus, given an approximation for $\tilde{\Gamma}$ the self-energy is completely defined through Eqs.(1-2) plus the Dyson equation for G . Electron-hole effects are embodied in the vertex function $\tilde{\Gamma}$ that appears in the self-energy directly, in Eq. (1), and through the polarization function, Eq. (2). The interplay between those two effects has been strongly debated in the last years, using different approximations for $\tilde{\Gamma}$, and different levels of self-consistency in the solution of Dyson equation. However all the systems analyzed in the past are characterized by moderate, if not absent, excitonic effects in the polarization function. Thus even if the use of two-point DFT-based [12, 13, 14] or finite order vertex functions $\tilde{\Gamma}$ [15] can be justified in the case of the homogeneous electron gas or simple semiconductors, they will be inadequate in the case of wide-gap insulators (e.g. LiF), as well as in the case of other strongly correlated systems. Next we derive a TDDFT approximation to the vertex function $\tilde{\Gamma}$ following the spirit of Ref. [5]: to reproduce the diagrammatic expansion of $\tilde{\Gamma}$ obtained within Many-body perturbation theory.

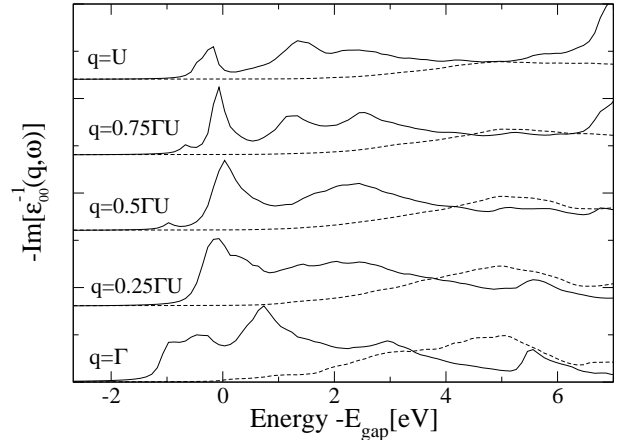


FIG. 2: Calculated loss function of LiF for momentum transfer \mathbf{q} along the direction ΓU . Continuous line: TDDFT calculation with an f_{xc} kernel that mimics excitonic effects [5]. Dashed line: RPA.

In the non self-consistent scheme the BSE expresses $\tilde{\Gamma}$ in terms of the independent particle W_0 (calculated using Eq. (2) assuming $\tilde{\Gamma}(1, 2; 3) = \delta(1, 2) \delta(1, 3)$) and the bare DFT Green’s function G_0 as:

$$\tilde{\Gamma}(1, 2; 3) = \delta(1, 2) \delta(1, 3) + iW_0(1, 2) \int d67 G_0(1, 6) G_0(7, 2) \tilde{\Gamma}(6, 7; 3). \quad (3)$$

When this vertex $\tilde{\Gamma}$ is inserted in Eq. (2), the corresponding equation for $\tilde{\chi}$ correctly describes excitonic effects in the polarization function at the BSE level [3]. Even if $\tilde{\Gamma}$ is an highly non-local, three-point function, it has been recently shown that, as long as we are interested in the two-point polarization function $\tilde{\chi}$, Eq. (2) can be cast in terms of the two-point exchange-correlation kernel f_{xc} of TDDFT [5, 16]:

$$\tilde{\chi}(1, 2) = \chi_0(1, 2) + \int d3 d4 \chi_0(1, 3) f_{xc}(3, 4) \tilde{\chi}(4, 2). \quad (4)$$

Here $\chi_0(1, 2) = -iG_0(1, 2)G_0(2, 1)$ gives the DFT polarization function. At this point if we take the exchange-correlation potential corresponding to f_{xc} as a local approximation to the self-energy, then the vertex function can be easily contracted into a two-point function: $\tilde{\Gamma}(6, 7; 3) \equiv \tilde{\Gamma}_{loc}(6, 3)\delta(6, 7)$ [12, 13, 14], with

$$\tilde{\Gamma}_{loc}(1, 2) = \left[\delta(1, 2) - \int d3 f_{xc}(1, 3) \chi_0(3, 2) \right]^{-1}. \quad (5)$$

Thus Eq. (1) gives $\Sigma(1, 2) = iW^{TDDFT}(1^+, 2)G_0(1, 2)$, in terms of the TDDFT effective potential $W^{TDDFT}(1, 2) = \int d3 v(1, 3) [\delta(3, 2) - \int d4 (v(3, 4) + f_{xc}(3, 4)) \chi_0(4, 2)]^{-1}$. From this self-energy the lifetime of a generic conduction state c with momentum \mathbf{k} is given by

$$\tau_{c\mathbf{k}}^{-1} = -2\Omega^{-1} \sum_{\mathbf{G}_1, \mathbf{G}_2} \sum_{\mathbf{q}, c'} \rho_{cc'}(\mathbf{k}\mathbf{q}\mathbf{G}_1) \rho_{cc'}^*(\mathbf{k}\mathbf{q}\mathbf{G}_2) \text{Im} [W_{\mathbf{G}_1\mathbf{G}_2}^{TDDFT}(\mathbf{q}, \epsilon_{c\mathbf{k}} - \epsilon_{c'\mathbf{k}-\mathbf{q}})], \quad (6)$$

with $\rho_{nn'}(\mathbf{k}\mathbf{q}\mathbf{G}) = \langle n\mathbf{k} | e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} | n'\mathbf{k}-\mathbf{q} \rangle$, \mathbf{G} a reciprocal space vector and Ω the crystal volume. Different expressions for $\tilde{\Gamma}_{loc}$, based either on local-field factor of the homogeneous electron gas [13] or on time-dependent local-density approximation (TDLDA) [12, 14] have shown that inclusion of local vertex corrections in both Σ and $\tilde{\chi}$ almost cancel out, i.e., $\tilde{\Gamma}_{loc}$ in Σ undresses the exchange-correlation effects included in the polarization function $\tilde{\chi}$. However such approximations for f_{xc} produce optical spectra very similar to RPA, in disagreement with experiments. This important drawback of a TDLDA f_{xc} has been recently related to the *long-range* nature of the kernel, $f_{xc}(\mathbf{r}, \mathbf{r}'; \omega) \sim -\alpha(\omega)/|\mathbf{r} - \mathbf{r}'|$ that partially counteracts the repulsive Hartree contribution [5, 16]. The stronger the electron-hole effects are, the larger is the correction embodied in α . In the case of wide-gap insulators like LiF there is a large region of frequencies and transfer momenta \mathbf{q} where f_{xc} is stronger than the Hartree term (i.e. $\alpha > 1$). This leads to unphysical linewidths: for a large energy range $\text{Im}(\Sigma)$, and hence τ^{-1} , has a wrong sign! This result is visualized by noticing that with respect to a G_0W_0 calculation a change of

sign of τ^{-1} is controlled by the *sign* ($v + f_{xc}$), that is proportional to $(1 - \alpha(\omega))$. A similar result was obtained in Ref. [12] looking at the high \mathbf{q} limit of the TDLDA kernel that goes as $f_{xc} \sim q^2$. The reason for this important failure of a two-point vertex function is connected to the imposed reduction of the non-locality from the original, three-point vertex function. In physical terms $\tilde{\Gamma}_{loc}$ overestimates the intensity of the vertex correction because two incoming particles (entering in 1 and 2 in the exact vertex function $\tilde{\Gamma}$) are supposed to coexist at the same time-space point. To overcome this difficulty we decided to release the constrain on the spatial locality and define a TDDFT vertex function $\tilde{\Gamma}_{TDDFT}(1, 2; 3)$ such that, for a given $f_{xc}(1, 2)$, $\tilde{\Gamma}_{TDDFT}$ is consistent with Eqs. (2-4). To this end we recall that in Ref. [5] we derived a diagrammatic expression for f_{xc} in terms of the screened coulomb potential W_0 , that to first order reads: $f_{xc} = \chi_0^{-1} \tilde{\chi}^{(1)} \chi_0^{-1}$, with $\tilde{\chi}^{(1)}$ the first order expansion of Eq. (2) in W_0 [17]. From this f_{xc} we get an approximation for the vertex function $\tilde{\Gamma}_{TDDFT}^{(1)}(1, 2; 3)$ imposing that once plugged in Eq. (2) it reproduces Eq. (4) for $\tilde{\chi}$. By inspecting Eqs. (2-4) we obtain

$$\tilde{\Gamma}_{TDDFT}^{(1)}(1, 2; 3) \equiv \delta(1, 2)\delta(2, 3) + iW_0(1, 2) \int d4 G_0(1, 4) G_0(4, 2) \tilde{\Gamma}_{loc}(4, 3), \quad (7)$$

It is crucial to observe that $\tilde{\Gamma}_{TDDFT}^{(1)}$ is *not* a first order vertex, as $\tilde{\Gamma}_{loc}$ sums an infinite number of diagrams. Eq. (7) can be easily generalized to give higher order approximations for $\tilde{\Gamma}$, consistent with the high order corrections to f_{xc} of Ref. [5]. As it is commonly done we neglect dynamical effects in the BSE [10], i.e. we assume $W_0(1, 2) \approx W_0(\mathbf{r}_1, \mathbf{r}_2; \omega = 0)$ in Eq. (7). This approximation is motivated in the present case, as we are interested in the low-energy electronic linewidths neglecting self-consistency effects. We have verified numerically that for LiF, Si, diamond and SiO₂ $\tilde{\Gamma}_{TDDFT}^{(1)}(1, 2; 3)$ is an excellent approximation to the “true” BSE vertex function $\tilde{\Gamma}$.

Now we can study the quasielectron lifetime in this approximation for the vertex function and for the electronic self-energy. To do so, we use as above the “on mass-shell” approximation, i.e., the lifetime is given by the imaginary part of $\Sigma = G_0 W \tilde{\Gamma}_{TDDFT}^{(1)}$ evaluated at the DFT energies:

$$\tau_{c\mathbf{k}}^{-1} = -\text{Im} [\langle c\mathbf{k} | \Sigma(\mathbf{r}, \mathbf{r}'; \epsilon_{c\mathbf{k}}) + \bar{\Sigma}(\mathbf{r}, \mathbf{r}'; \epsilon_{c\mathbf{k}}) | c\mathbf{k} \rangle]. \quad (8)$$

Here the linewidths are computed as an average of the “left” and “right” self-energies, Σ and $\bar{\Sigma}$ [9] in order to restore the proper \mathbf{r}, \mathbf{r}' symmetry of the self-energy. Using Eq. (7) $\tau_{c\mathbf{k}}^{-1}$ can be simplified by performing the energy integration in the complex plane and exploiting the pole

structure of $\tilde{\Gamma}_{TDDFT}^{(1)}$:

$$\begin{aligned} \tau_{\mathbf{ck}}^{-1} &= \tau_{\mathbf{ck},0}^{-1} \\ &- 2\Omega^{-1} \sum_{\mathbf{G}_1, \mathbf{G}_2} \sum_{\mathbf{q}, \mathbf{c}'} \text{Im} [W_{\mathbf{G}_1 \mathbf{G}_2}^{TDDFT}(\mathbf{q}, \epsilon_{\mathbf{ck}} - \epsilon_{\mathbf{c}'\mathbf{k}-\mathbf{q}})] \\ &\text{Re} [(\Gamma_{\mathbf{cc}'}^{cv}(\mathbf{kqG}_1) + \Gamma_{\mathbf{cc}'}^{vc}(\mathbf{kqG}_1)) \rho_{\mathbf{cc}'}^*(\mathbf{kqG}_2)], \quad (9) \end{aligned}$$

where $\tau_{\mathbf{ck},0}^{-1}$ corresponds to the standard G_0W approximation, and

$$\begin{aligned} \Gamma_{\mathbf{cc}'}^{cv}(\mathbf{kqG}) &= \Omega^{-1} \sum_{\mathbf{G}_1 \mathbf{G}_2} \sum_{\mathbf{Q} c_2 v_2} \rho_{\mathbf{cc}_2}(\mathbf{kqG}_1) [W_0(\mathbf{Q})]_{\mathbf{G}_1 \mathbf{G}_2} \\ &\rho_{\mathbf{c}'v_2}^*(\mathbf{k}-\mathbf{qQG}_2) \rho_{\mathbf{c}_2 v_2}(\mathbf{k}-\mathbf{QqG}) \\ &(\epsilon_{\mathbf{ck}} - \epsilon_{\mathbf{c}'\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{c}_2 \mathbf{k}-\mathbf{Q}} + \epsilon_{\mathbf{v}_2 \mathbf{k}-\mathbf{q}-\mathbf{Q}})^{-1}, \quad (10) \end{aligned}$$

$$\begin{aligned} \Gamma_{\mathbf{cc}'}^{vc}(\mathbf{kqG}) &= \Omega^{-1} \sum_{\mathbf{G}_1 \mathbf{G}_2} \sum_{\mathbf{Q} c_2 v_2} \rho_{\mathbf{cv}_2}(\mathbf{kqG}_1) [W_0(\mathbf{Q})]_{\mathbf{G}_1 \mathbf{G}_2} \\ &\rho_{\mathbf{c}'c_2}^*(\mathbf{k}-\mathbf{qQG}_2) \rho_{\mathbf{v}_2 c_2}(\mathbf{k}-\mathbf{QqG}) \\ &(\epsilon_{\mathbf{ck}} - \epsilon_{\mathbf{c}'\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{v}_2 \mathbf{k}-\mathbf{Q}} + \epsilon_{\mathbf{c}_2 \mathbf{k}-\mathbf{q}-\mathbf{Q}})^{-1}. \quad (11) \end{aligned}$$

Eq. (9) constitutes the main basic result of this communication, and can be easily extended to the quasihole linewidths. Eq. (6) must be compared with Eq. (9). In the case of weakly interacting systems the two equations with a TDLDA f_{xc} give very similar quasiparticle corrections to the gap and electron linewidths [12, 13, 14]. But, as short-range correlations become important Eq. (6) tends to give non-sensible results (negative linewidths) because of the wrong sign of W^{TDDFT} . In Eq. (9), instead, the term $(\Gamma_{\mathbf{cc}'}^{cv} + \Gamma_{\mathbf{cc}'}^{vc})$ reflects the spatial non-locality of $\tilde{\Gamma}_{TDDFT}^{(1)}$ strongly reducing the weight of W^{TDDFT} . Consequently the final expression for $\tau_{\mathbf{ck}}^{-1}$ is given by $\tau_{\mathbf{ck},0}^{-1}$ plus a small vertex correction that does not change appreciably the results of a simpler G_0W calculation. The fundamental practical result of this work corresponds to the solution of Eq. (9) for LiF, shown in Fig. 1. The overall effect of excitons in the linewidths is huge [18]: the linewidths up to 3 eV above the forbidden region display a linear dependence with energy while the RPA are almost zero because of the slow rise of the RPA loss function (see Fig. 2). A similar energy dependence has been observed in highly correlated materials [8]. Instead the present linear dependence of the linewidths is due to the combination of an almost constant density-of-states close to the conduction band minimum and to a “step-like” energy dependence of loss function (see Fig. 2). Furthermore, the quasiparticle linewidths are not exactly zero in a small energy window of 0.5 eV in the forbidden region. This effect can be traced back to the excitonic-induced transfer of oscillator strength in the dynamical dielectric function *below* the gap. This result is consistent with the fact that exciton dynamics is dictated by vertex-correction to the self-energy, therefore

an interpretation of the quasiparticle scattering based only on independent-particle processes loses meaning. The results of the present work allow for the systematic analysis of the role of excitons in quasiparticle excitations and response functions of extended and low dimensional systems, where the standard G_0W_0 approximation fails [2, 3].

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